Hexyl acetate 142-92-7 | DTXSID6022006

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Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 1.75 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.30e-01

Confidence level: 7.77e-01

Nearest Neighbors from the Training Set

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Hexadecanoic acid, 1methylethyl ester Measured: 1.32 Predicted: 2.42e-05

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Methyl valerate Measured: 3.60 Predicted: 15.6

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2-Ethoxyethanol Measured: 5.40e-01 Predicted: 5.91

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2-tert-Butyl-4-ethylphenol

Measured: 2.12 Predicted: 2.17e-02